Appendix C
Vadose Zone Data for Initial Assessment Performed with the
System Assessment Capability (Revision 0)

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1.0   Introduction

This report describes the data compiled in Fiscal Years 2000 and 2001 to support Vadose Zone modeling in the initial assessment performed using the System Assessment Capability (Revision 0). The requirements and design of the SAC Rev. 0 and a description of the initial assessment are presented in the *System Assessment Capability (Revision 0), Assessment Description, Requirements, Software Design, and Test Plan* document (Kincaid et al., 2000). Background information on the development of the SAC is presented in *Preliminary System Assessment Capability Concepts for Architecture, Platform and Data Management*[1] and Kincaid et. al. (2000).

The purpose of this activity was to gather all data and interpreted information needed to define the physical and geochemical parameters for the vadose zone simulations conducted as part of the initial assessment. Much of these data were extracted from existing documents and databases and the appropriate references are provided where available.

2.0   Background

Kincaid et al. (2000) specified that the vadose zone flow and transport simulations for the initial assessment would be based on 1) hydrogeologic profiles and properties for aggregate release areas, 2) estimates of deep infiltration (i.e. recharge) rates, 3) estimates of geochemical reactions, and (4) waste inventory and release projections. The first three of these data types are supplied in this report. The fourth, waste inventory and release projections, is supplied by their respective technical elements. The vadose zone profile and property models for the initial assessment are

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[1] These documents can be found at http://www.bhi-erc.com/vadose/sac.htm#info

represented by a single generalized one-dimensional vertical column for each of 13 aggregate areas (Figure 2.1).

Kincaid et al. (2000) identified the Subsurface Transport Over Multiple Phases (STOMP) computer code (White and Oostrom, 1996) as the code of choice for the Vadose Zone Flow and Transport Module for SAC Rev. 0. SAC Rev. 0 simulates intentional liquid discharges to 689 individual sites but aggregates 201 dry-waste burial grounds and unplanned releases into 30 aggregate sites based on their location, waste release model, and waste chemistry designations. This yields a total of 719 sites to be simulated.

The original plan called for a single hydrostratigraphic template to represent the soil column for a single aggregate area. Each individual template would be configured with the hydraulic and geochemical parameters necessary for STOMP to simulate the flow and transport through the vadose zone. However, it was later realized that as many as four variations of a single template were necessary to more accurately represent the depth of waste releases and the thickness of the vadose zone beneath the point of injection. It was also recognized that additional variations of the templates might be necessary to accommodate the variations in K_ds associated with different waste chemistry designations. Thus, a series of 64 base templates were ultimately identified for application in the 13 aggregate areas shown in Figure 2.1. These base templates consist of the one-dimensional stratigraphy, hydrologic properties, and geochemical properties as well as the waste site type (e.g. crib, tank, etc.) and waste chemistry designation. A more complete discussion regarding the development of the 64 base templates is provided in Section 4.1.

The preferred approach (and the rational behind it) for modeling contaminant transport through the vadose zone for SAC Rev. 0 (is presented in *Preliminary System Assessment Capability Concepts for Architecture, Platform and Data Management*[1]). This approach uses these base templates to represent the vadose zone beneath each waste site within a given aggregate area. However, the actual simulation of each waste site assigned to a given template (see Section 4.2) is implemented at the site's centroid coordinates, not at coordinates for the entire template.

Each base template consists of a few major hydrostratigraphic units that are of uniform thickness, horizontal, homogeneous and isotropic (Figure 2.2). Hydrologic and geochemical parameters for each hydrostratigraphic unit are represented by stochastic distributions to facilitate sensitivity and uncertainty analyses. Once each site was assigned to an aggregate area and representative base template, site-specific parameters such as the site location (centroid), soil column area (foot print and/or affected [wetted] column area [i.e. account for lateral spreading]), and recharge rates (based on surface cover changes) were added. Each site (either a separate liquid disposal site or an aggregation of several dry waste or unplanned release sites) was then assigned a unique alphanumeric identifier.
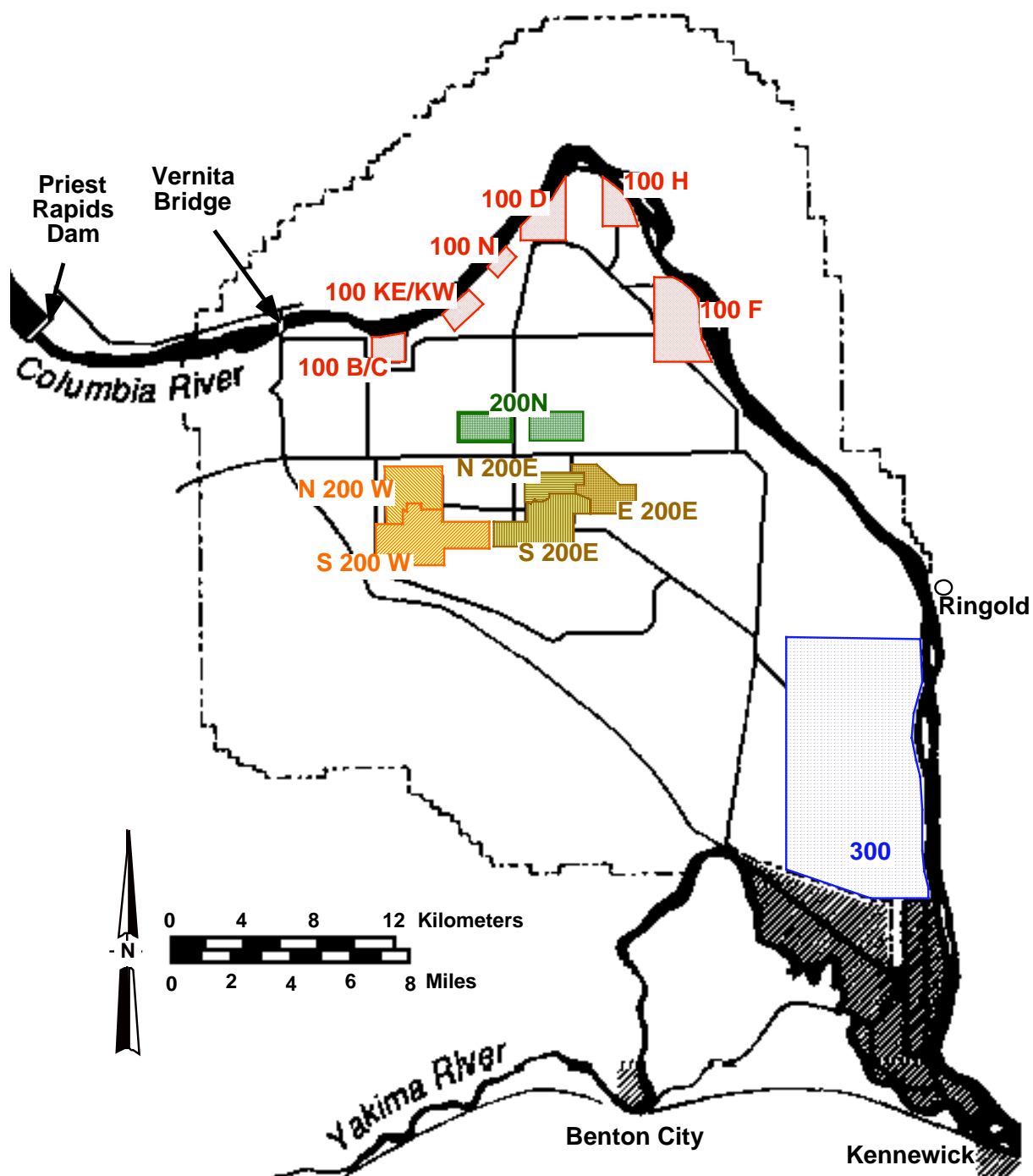
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[1] These documents can be found at http://www.bhi-erc.com/vadose/sac.htm#info

Figure 2.1. Location of Aggregate Areas To Be Represented by a Single Generalized Stratigraphic Column.

Q_I

Q_I = Mass Flux to Vadose Zone from Release Model

Infiltration through surface cover

R = Column width, which is equal to the square root of the WIDS facility area * a multiplication factor for large volume disposals

Hydrostratigraphic column dependent on number and thickness of major hydrostratigraphic units

Q_O = Mass Flux to Groundwater
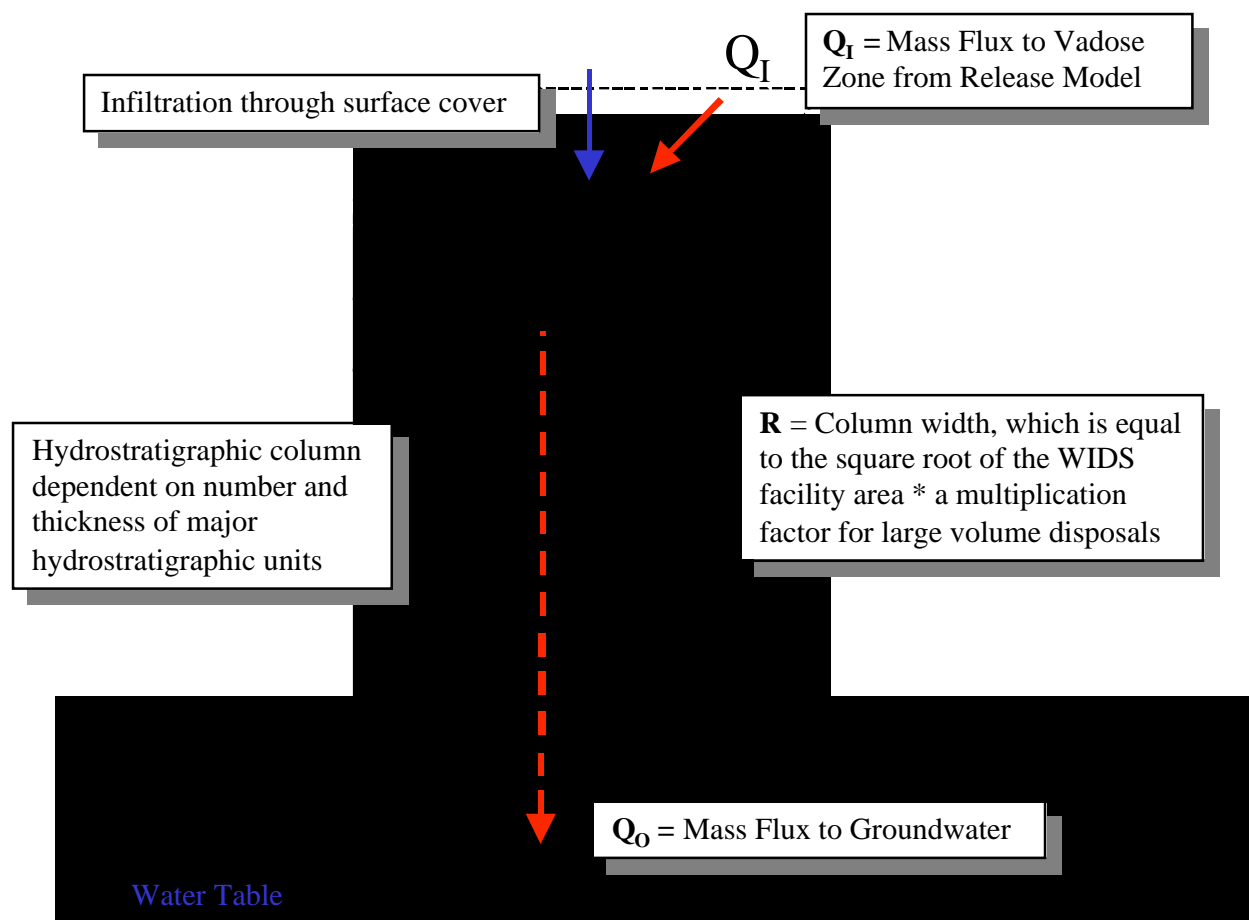
Water Table

Figure 2.2. Schematic of One-Dimensional Vadose Zone Simulation

3.0   Vadose Zone Module Interaction with the Inventory, Release, and Groundwater Modules

The inventory and release modeling results for the initial assessment provide input to the vadose zone module. In addition to curie or kilogram amounts of waste and waste volume, the inventory module provides data on the location and dimensions of each storage or disposal facility. The release module, in concert with the inventory module, provides the contaminant flux to the vadose zone. Large-volume contaminant releases to sites where the vadose zone is thin, such as the cooling water discharges to retention basins in the 100 areas, are routed directly to the Columbia River, bypassing the vadose zone. Contaminant flux out of the Vadose Zone module is used as input to the groundwater module.

4.0   Vadose Zone Data Gathering

Data gathering efforts for the vadose zone technical element were conducted in two general phases; 1) definition of the base templates, and 2) definition of the site-specific templates.

4.1   Base Templates

Sixty-four base templates were defined on the basis of 1) the type of waste site, 2) the aggregate area (geographic area/geology [Figure 2.1]), and 3) the characteristics of the waste stream. To accommodate the large number of templates, a six digit (alphanumeric) code was developed to identify each unique base template. This code consists of a 3 digit number to reflect the waste site type, a letter designating the aggregate area, and a number designating the waste chemistry group for assigning K_ds. These codes are explained below.

4.1.1 Waste Site Type (Reflecting the Depth of Waste Injection)

Nearly all waste sites selected for simulation in the initial assessment have a Waste Information Data System (WIDS) site code, This code generally includes a three digit number, with the first digit identifying the area where the facility is located, and the second and third digits identifying the type of facility it is. For example the site code that includes the digits 116 indicates that the facility is in the 100 Area and that it is a liquid disposal facility (i.e. crib, pond, ditch, etc.); a site code with the digits 241 indicates that it is in the 200 Area and that it is a underground high-level waste tank. For the purposes of defining the base templates, four main categories of waste site type were distinguished: 1) surface facilities (e.g. ponds, ditches, retention basins, buildings, unplanned releases), 2) near surface facilities (e.g. cribs, specific retention trenches, French drains, burial grounds), 3) underground storage tanks, and 4) reverse (injection) wells. Each of these site types release waste to the vadose zone at increasingly deeper depths, making the stratigraphic column shorter, and moving the location of high impact vs. intermediate impact K_d zones deeper in the soil profile. The waste site designation scheme for implementation in the base template nomenclature is shown in Table 4.1.

Table 4.1. Waste Site Type Designations used in the Base Template Codes

Waste Site Type Designation[1]	Facility Types (Reflecting Depth of Waste Injection)
100, 200, 300	Surface or near surface facilities (e.g. process sewers, reactor buildings, laboratory buildings, stacks, ponds, ditches, valve pits, process plants, unplanned releases [except tank leaks]).
116, 216, 316	Shallow liquid and/or dry waste disposal facilities (e.g. cribs, burial grounds, retention basins, trenches, French drain, storage tunnels, drain/tile fields.
241	High level waste tanks, settling tanks, diversion boxes, catch tanks, tank leak unplanned releases.
266, 276	Deep injection sites (e.g. reverse wells)

[1] First digit represents the area: 1 = 100 Area, 2 = 200 Area, 3 = 300 Area. Second and third digits indicate the facility type.

4.1.2 Aggregate Areas

Thirteen aggregate areas (Figure 2.1) were defined based on geographically contiguous areas with relatively homogeneous hydrogeologic characteristics. Each of the six 100 Areas were designated as separate aggregate areas because each area is geographically distinct and have distinct hydrogeologic characteristics. The 200 Areas were divided into six aggregate areas

based on differences in hydrogeologic characteristics. The 200 West and 200 East Areas were each divided into two aggregate areas. Additional aggregate areas were designated for the 200 North/Gable Mountain Pond area, and the B-Pond area. Finally, a single aggregate area was designated to encompass waste sites in the 300 Area, and four isolated sites in and around the 400 area. Table 4.2 presents the letter designations and brief descriptions of each aggregate area.

Table 4.2. Aggregate Area Designations used in the Base Template Codes

Designation	Aggregate Area Description
A	Southern 200 East Area - encompassing the PUREX (**A** plant), Hot Semi-Works (C-Plant), associated facilities (including PUREX tunnels), BC cribs, US Ecology, and the A, AN, AP, AW, AX, AY, AZ, C Tank Farms
B	Northwestern 200 East Area - encompassing the **B**-plant Area, associated waste disposal facilities, and the B, BX, BY Tank Farms
C	100-B/**C** Area
D	100-**D**/DR Area
E	**E**ast of 200 East - B-pond Area
F	100-**F** Area
G	200 North and **G**able Mountain Pond Areas
H	100-**H** Area
K	100-**K**E/KW Area
N	100-**N** Area
R	300 Area (and a few isolated facilities in and near the 400 Area)
S	Southern 200 West Area - encompassing the REDOX (**S**-Plant), U-plant, Z-plant associated facilities, ERDF, and the S, SX, SY, U Tank Farms
T	Northern 200 West Area - encompassing **T** Plant , associated facilities, and the T, TX, TY Tank Farms

4.1.3 Waste Chemistry Groupings (for assigning Kd ranges)

Six waste chemistry types were defined by Kincaid et al (1998) for use in the Composite Analysis. These waste chemistry types describe chemically distinct waste streams that impact the sorption of contaminants. These same waste chemistry designations were adapted for use in the initial assessment to assign Kd values to the vadose zone base templates. Table 4.3 describes the waste chemistry designations.

Table 4.3. Waste Chemistry Designations used in the Base Template Codes

Waste Chemistry Designation	Waste Stream Description
1	High Organic / Very Acidic
2	High Organic / Near Neutral
3	High Salt / Very Basic
4	Chelates / High Salt
5	Low Organic / Low Salt / Acidic
6	Low Organic / Low Salt / Near Neutral

4.1.4 Base Template Designations

A total of 64 base templates have been identified based on various combinations of the aggregate areas, site types, and waste chemistry types. Table 4.4 provides a description of each base template.

Table 4.4. List of Base Templates for SAC Rev. 0 Vadose Zone Modeling

Base Template Designation	Aggregate Area		Waste Site Types		Waste Chemistry Designation
	Area	Designation[1]	Description	Designation[2]	
100C-6	100 B/C	C	Surface Facilities	100	6
116C-6			Near Surface Facilities	116	6
100D-6	100 D	D	Surface Facilities	100	6
116D-6			Near Surface Facilities	116	6
100F-6	100 F	F	Surface Facilities	100	6
116F-6			Near Surface Facilities	116	6
100H-6	100 H	H	Surface Facilities	100	6
116H-6			Near Surface Facilities	116	6
100K-6	100 K	K	Surface Facilities	100	6
116K-6			Near Surface Facilities	116	6
166K-5			Reverse Wells	166	5
166K-6					6
100N-5	100 N	N	Surface Facilities	100	5
100N-6					6
116N-6			Near Surface Facilities	116	6
200G-6	200N/Gable	G	Surface Facilities	200	6
216G-6	Mountain Pond		Near Surface Facilities	216	6
200E-6	E 200 E (B-Pond)	E	Surface Facilities	200	6
200B-3	N 200 E (B-Plant)	B	Surface Facilities	200	3
200B-4					4
200B-6					6
216B-3			Near Surface Facilities	216	3
216B-4					4
216B-6					6
241B-3			Tanks	241	3
267B-3			Reverse Wells	267[3]	3
266B-6				266	6
200A-3	S 200 E (PUREX,	A	Surface Facilities	200	3
200A-6	BC Cribs)				6
216A-2			Near Surface Facilities	216	2
216A-3					3
216A-4					4
216A-5					5
216A-6					6
241A-3			Tanks	241	3
241A-4					4
266A-6			Reverse Wells	266	6
200S-1	S 200 W (Redox, U-	S	Surface Facilities	200	1
200S-2	Plant, Z-Plant)				2
200S-3					3
200S-5					5
200S-6					6

Base Template Designation	Aggregate Area		Waste Site Types		Waste Chemistry Designation
216S-1	S 200 W (Redox, U-Plant, Z-Plant)	S	Near Surface Facilities	216	1
216S-2					2
216S-3					3
216S-5					5
216S-6					6
241S-2			Tanks	241	2
241S-3					3
241S-6					6
266S-6			Reverse Wells	266	6
200T-3	N 200 W (T-Plant)	T	Surface Facilities	200	3
200T-6					6
216T-2			Near Surface Facilities	216	2
216T-3					3
216T-4					4
216T-5					5
216T-6					6
241T-3			Tanks	241	3
266T-3			Reverse Wells	266	3
266T-5					5
300R-5	300 Area (North Richland	R	Surface Facilities	300	5
300R-6					6
316R-6			Near Surface Facilities	316	6

[1] Assigned letter designation for aggregate area.

[2] Assigned number designation for waste site type: First number designates traditional Hanford Site area (i.e. 100, 200, 300 Areas); last two numbers designate waste site type (00 = surface facilities, 16 = near surface facilities, 41 = tanks, 66/67 = reverse wells)

[3] Two designations are use for reverse wells that have very different depths within a single aggregate area. The "67" designation distinguishes the very deep reverse wells from those at a more intermediate depth (66).

4.1.5 Hydrostratigraphy

Generalized hydrostratigraphic columns were specified for each of the 13 aggregate areas. These columns were assembled from existing information including:

- driller's logs, geologists' logs, and geophysical logs
- published interpretive depths to the top and bottom surfaces of hydrogeologic units
- surface elevations (to convert hydrogeologic unit depths to elevations)
- elevation of the 1944 water table (to define the bottom of the vadose zone prior to waste disposal).

Table 4.5 lists the published references used to assign hydrogeologic units to each base template.

The generalized hydrostratigraphic units used in this study are briefly described in Table 4.6. In general, the depth and thickness of each hydrogeologic layer (strata) for each aggregate area were taken from published maps and cross-sections. The estimated average strata thickness was used for the generalized columns extending from the surface to the 1944 water table (Kipp and Mudd, 1973). Because the sum of the average thicknesses did not always equal the distance from the surface to the water table, small adjustments were made to the average strata thicknesses. Attachment 1 illustrates the hydrostratigraphic column for each aggregate area, including the layer thicknesses, and their hydraulic and geochemical property designations.

Table 4.5. Sources of Hydrogeologic Data

Aggregate Area	References
100 B/C	Lindberg, 1993; Lindsey, 1992; Peterson et al., 1996
100 D	Lindsey and Jaeger, 1993,; DOE, 1993d; Lindsey, 1992; Peterson et al., 1996
100 F	Raidl, 1994; Lindsey, 1992; Peterson et al., 1996
100 H	Lindsey and Jaeger, 1993; Liikala et al., 1988; Vermuel et al., 1995; DOE/RL, 1993d; Peterson et al., 1996
100 K	Lindsey, 1992; Lindberg, 1995; Peterson et al., 1996
100 N	Hartman and Lindsey, 1993
200 North / Gable Mountain Pond Area	Lindsey et al., 1992b; DOE, 1993a; DOE, 1993b; Wurstner et al., 1995
E 200 E (B-Pond)	Barnett et al., 2000; Clearlock et al., 2000; Lindsey et al., 1992b; Wurstner et al., 1995
N 200 E (B-Plant)	Lindsey et al., 1992b; Price and Fecht, 1976b; Price and Fecht, 1976c; Price and Fecht, 1976d; Tallman et al., 1979; Wurstner et al., 1995; Wood et al., 2000
S 200 E (PUREX, BC cribs)	Lindsey et al., 1992b; Reidel and Horton, 1999; Tallman et al., 1979; Wurstner et al., 1995
S 200 W (Redox, U-Plant, Z-Plant)	Johnson and Chou, 1988; Lindsey et al. 1992a; Price and Fecht, 1976a; Slate, 2000; Tallman et al., 1979; Wurstner et al., 1995; Rohay, et al., 1994
N 200 W (T-Plant)	Lindsey et al., 1992a; Slate, 2000; Tallman et al., 1979; Wurstner et al., 1995
300 Area (North Richland)	Gaylord and Poeter, 1991; Lindberg and Bond, 1979; Schalla et al., 1988; Swanson et al., 1992

Table 4.6. Summary of hydrostratigraphic units used in this study

Formation	Facies / Subunit	Description
NA	Backfill	Poorly sorted gravel, sand, and silt derived from the Hanford formation and/or Holocene deposits
Holocene	Eolian	Dune sand and silt
Hanford formation	Silt-dominated	Interbedded silt and fine to coarse sand
	Sand-dominated	Stratified fine to coarse sand with minor pebbles and minor laterally discontinuous silt interbeds
	Gravelly Sand	Cross bedded, interstratified coarse sand with up to 30 wt% very fine pebble to cobble
	Gravel-Dominated	Cross bedded, interstratified coarse sand and gravel with greater than 30 wt% very fine pebble to boulder
	Undifferentiated	Undifferentiated sand and gravel with minor discontinuous silt interbeds.
Plio-Pleistocene Unit	Silt/Sand Dominated	Very Fine Sand to Clayey Silt Sequence. Interstratified silt to silty very fine sand and clay deposits
	Carbonate Rich	Carbonate-Rich Sequence. Weathered and naturally altered sandy silt to sandy gravel, moderately to strongly cemented with secondary pedogenic calcium carbonate.
Ringold Formation	Fluvial Sand (Member of Taylor Flat)	Interstratified sand and silt deposits
	Fluvial Gravel (Member of Wooded Island, subunit E)	Moderate to strongly cemented well rounded gravel and sand deposits, and interstratified finer-grained deposits.
	Overbank/Lacustrine Deposits (Lower Mud Sequence)	Predominantly mud (silt and clay) with well developed argillic to calcic paleosols.

4.1.6 Hydraulic Properties

Hydraulic property data were primarily taken from Khaleel and Freeman (1995) as supplemented by Khaleel (1999), Khaleel, et. al. (2000), and an informal letter report.[1] Because this data set is

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[1] Khaleel, R. September 2000. Vadose Zone Hydraulic Parameter Estimates for S-SX SAC Rev. 0 Models.

rather limited in regards to the spatial location of samples and the soil types represented, individual stochastic data sets were selected to represent each hydrogeologic strata present in the 13 aggregate areas. Care was taken to ensure that the soil classifications for which hydraulic property data was available, could be correlated to the sediment facies within each template. Relationships between hydrostratigraphic units and the soil classifications for which hydraulic property data were developed are shown in Table 4.7.

The statistical distributions of van Genuchten model (van Genuchten 1980) parameters, saturated hydraulic conductivity, and bulk density data were taken primarily from Khaleel and Freeman (1995) and Khaleel, et. al. (2000). Those for longitudinal dispersivity were primarily taken from Ho, et. al. (1999). Values for residual saturation (S_r) were calculated by dividing the raw residual water content (θ_R) by the raw saturated content (θ_S), as provided by Khaleel and Freeman (1995). Effective porosity is assumed to be equal to the saturated water content (θ_s). Table 4.8 shows the hydraulic properties and their estimated stochastic distributions assigned to each designation.

Note that all model nodes within a single hydrogeologic unit are assigned the same hydraulic properties for a single realization. Initial truncation limits for the stochastic distributions were chosen based on the extreme mimima and maxima of observed data (stochastic sampling of parameters is restricted to within specified truncation limits in the SAC software). Iterative testing demonstrated the need for further truncation on the lower bound of the van Genuchten *n* and saturated hydraulic conductivity parameters. It was found that the sampling of the saturated hydraulic conductivity distributions should be truncated at a lower limit of 35 percent, and van Genuchten's exponent *n* parameter should be truncated at a lower limit of 25 percent. All other parameters are restricted to the maximum observed data range for their distributions. Application of these truncation limits greatly reduces (but does not eliminate) the "failure rate" for vadose zone calculations in SAC Rev. 0. It should be noted that these truncations limits on conductivity and van Genuchten's n are "conservative" in that they overestimate rather than underestimate releases from the vadose zone.

Note also that the Vadose Zone Expert Panel identified colloid-facilitated transport and preferential flow (caused in part by thermal and density effects) as potentially important processes (DOE 1997). However, our simplified 1-D transport modeling approach for SAC Rev. 0 neglects these processes.[2]

Table 4.7. Correlation between Hydrostratigraphic Units and Soil Classifications used for Hydraulic Property Designation

Hydrostratigraphic Unit	Hydraulic Property Designation	Soil Classification Description[1]
• Backfill	B	Backfill
• Holocene eolian deposits • Hanford formation sand	S	Sand

[2] Groundwater/Vadose Zone Integration Project. Preliminary System Assessment Capability Concepts for Architecture, Platform, and Data Management. September 30, 1999.

Hydrostratigraphic Unit	Hydraulic Property Designation	Soil Classification Description[1]
• Ringold Formation sand (i.e. Wooded Island member)		
• Hanford formation gravelly sand	GS	Gravelly sand
• Hanford formation gravel • Undifferentiated Hanford deposits • Undifferentiated Hanford/coarse Plio-pleistocene deposits	SG1	Sandy gravel with gravel fraction < 60 %
• Old Hanford/Plio-Pleistocene ("Early Palouse") • Plio-Pleistocene Caliche • Ringold Formation Lower Mud	SS	Sand mixed with finer fraction
• Ringold Formation Unit E	SG2	Sandy gravel with gravel fraction > 60 %

[1] Information from Khaleel and Freeman, 1995.

4.1.7 Distribution Coefficients

Geochemical properties were assigned to each hydrogeologic unit, in a manner similar to that done for the Composite Analysis (Kincaid et. al., 1998). The waste characteristics were assumed to dominate the near-field mobility of the contaminants in the vadose zone. After being in contact with vadose zone sediments and soil water for some distance, the waste undergoes a change in its mobility based on buffering of the contaminant solution by the vadose zone sediments. Thus, distribution coefficients were defined separately for each contaminant in the upper vadose zone [near field or high impact zone] and in the lower vadose zone [far field or intermediate impact zone] (Kincaid et. al., 1998).

Distribution coefficient zones were defined as either high impact or intermediate impact depending on the nature of the contamination fluid. Zones in which the organic concentration, pH, or salt concentration in the fluids may have affected the K_d values were designated high-impact. Zones in which the acidic or basic nature of the wastes was estimated to have been neutralized by the natural soil were designated intermediate-impact. Kincaid et. al. (1998) estimated the depths of this transition zone by examining the peak location of beta/gamma contamination (as presented by Fecht et. al., 1977) for 200 Area cribs receiving very acid or high-salt/very basic waste. In general these transition depths ranged from 10 to 40 meters. Given the limited data available on which to base further interpretations on the depths of transition, and the desire to simplify the numerical simulations, a slightly different approach was used here. Generally, the hydrogeologic unit into which waste streams were introduced was designated as high-impact regardless of waste stream characteristics. If those hydrogeologic units were thin, then the hydrogeologic unit immediately below that into which the waste stream was introduced was also designated high-impact. All other hydrogeologic units lower in the profile were designated intermediate impact. This approach enabled us to keep the numerical simulations relatively simple by using the existing number of hydrogeologic units (i.e., we did not have to add new layers to make the K_d change where it might have occurred within a single hydrogeologic unit). At the same time, the depths of change, corresponding to the thickness of the hydrogeologic units, are still on the same scale (tens of meters) as those used by Kincaid et.

al. (1998). Attachment 1 provides the detailed hydrogeologic columns and locations of the various K_d zones, for each base template.

Table 4.8. Hydraulic Property Distributions for the van Genuchten/Mualem Model

Backfill - based on Khaleel and Freeman (1995) soil category SSG (sand and gravel mixed with finer fraction)

Parameter	Number of samples	Raw				Transform	Transformed (normal distribution)				Beta Distribution	
		Low	High	Mean	Std Deviation		Upper Limit	Lower Limit	Mean	Std Deviation	A	B
Sat. Moist. Content (θ_s)[*][3]	6	0.187	0.375	0.262	0.072	NO	-	-	-	-	-	-
Res. Moist. Content (θ_r)[*]	6	0	0.064	0.03	0.029	NO	-	-	-	-	-	-
Res. Saturation (S)[**]	7	0	0.213	0.102	0.0895	BETA					1.0572	9.3483
Van Genuchten α (1/cm)	6	0.003	0.103	0.032	0.036	LN	-5.843	-2.276	-3.957	1.166	-	-
Van Genuchten n	6	1.256	1.629	1.4	0.131	NO	-	-	-	-	-	-
Sat. Conductivity (K_s)(cm/s)	6	0.0000276	0.068	0.015	0.027	LR	-10.854	2.995	-5.262	5.499	-	-
Longitudinal Dispersivity (m)	NA	2.70E-02	0.178	0.09	NA	UN	-	-	-	-	-	-
Bulk Density[2]	NA	-	-	1.94	-	CO	-	-	-	-	-	-

Holocene eolian sand, Hanford sand, and Ringold sand - based on Khaleel and Freeman (1995) soil category S (sand)

Parameter	Number of samples	Raw				Transform	Transformed (normal distribution)				Beta Distribution	
		Low	High	Mean	Std Deviation		Upper Limit	Lower Limit	Mean	Std Deviation	A	B
Sat. Moist. Content (θ_s)[*][3]	76	0.197	0.519	0.346	0.073	NO	-	-	-	-	-	-
Res. Moist. Content (θ_r)[*]	76	0	0.148	0.029	0.023	SN	0	0.881	0.189	0.146	-	-
Res. Saturation (S)[**]	80	0	0.445	0.086	0.0685	BETA					1.3694	14.4639
Van Genuchten α (1/cm)	76	0.004	0.861	0.108	0.164	LN	-5.547	-0.149	-3.097	1.347	-	-
Van Genuchten n	76	1.193	4.914	2.111	0.817	LR	-5.756	4.33	-1.459	1.523	-	-
Sat. Conductivity (K_s)(cm/s)	71	1.38E-05	5.80E-02	6.00E-03	1.10E-02	LN	-11.191	-2.847	-6.849	2.129	-	-
Longitudinal Dispersivity (m)	NA	1.83E-01	0.223	0.203	NA	UN	-	-	-	-	-	-
Bulk Density[2]	NA	-	-	1.76	-	CO	-	-	-	-	-	-

Hanford gravelly sand - based on Khaleel and Freeman (1995) soil category GS (gravelly sand).

Parameter	Number of samples	Raw				Transform	Transformed (normal distribution)				Beta Distribution	
		Low	High	Mean	Std Deviation		Upper Limit	Lower Limit	Mean	Std Deviation	A	B
Sat. Moist. Content (θ_s)[*][3]	10	0.203	0.334	0.272	0.048	NO	-	-	-	-	-	-
Res. Moist. Content (θ_r)[*]	10	0.01	0.069	0.04	0.019	NO	-	-	-	-	-	-
Res. Saturation (S)[**]	9	0.030	0.244	0.157	0.0713	BETA					3.9262	21.0801
Van Genuchten α (1/cm)	10	0.004	0.074	0.027	0.023	NO	-	-	-	-	-	-
Van Genuchten n	10	1.529	2.537	1.994	0.315	NO	-	-	-	-	-	-
Sat. Conductivity (K_s)(cm/s)	10	5.43E-05	8.00E-03	3.00E-03	3.00E-03	LR	-7.966	2.989	-1.569	3.582	-	-
Longitudinal Dispersivity (m)	NA	4.68E-02	0.134	0.088	NA	UN	-	-	-	-	-	-
Bulk Density[2]	NA	-	-	2.07	-	CO	-	-	-	-	-	-

Hanford gravel and undifferentiated Hanford and coarse Plio-pleistocene deposits - based on Khaleel and Freeman (1995) soil category SG1 (sandy gravel with gravel < 60%).

Parameter	Number of samples	Raw				Transform	Transformed (normal distribution)				Beta Distribution	
		Low	High	Mean	Std Deviation		Upper Limit	Lower Limit	Mean	Std Deviation	A	B
Sat. Moist. Content (θ_s)[*][3]	25	0.113	0.26	0.166	0.036	NO	-	-	-	-	-	-
Res. Moist. Content (θ_r)[*]	25	0	0.062	0.023	0.015	NO	-	-	-	-	-	-
Res. Saturation (S)[**]	26	0	0.387	0.131	0.0925	BETA					1.6221	10.7165
Van Genuchten α (1/cm)	25	0.002	0.919	0.083	0.204	LN	-6.075	-0.084	-4.086	1.55	-	-
Van Genuchten n	25	1.262	2.947	1.66	0.355	LN	0.233	1.081	0.489	0.184	-	-
Sat. Conductivity (K_s)(cm/s)	24	1.90E-07	3.70E-02	5.00E-03	9.00E-03	LN	-15.476	-3.297	-7.932	3.322	-	-
Longitudinal Dispersivity (m)	NA	0.027	0.178	0.09	NA	UN	-	-	-	-	-	-
Bulk Density[2]	NA	-	-	2.07	-	CO	-	-	-	-	-	-

Undifferentiated Hanford/fine-grained Plio-Pleistocene (Early Palouse Soil), Plio-Pleistocene caliche, and Ringold mud - based on Khaleel and Freeman (1995) soil category SS (sand mixed with finer fraction).

Parameter	Number of samples	Raw				Transform	Transformed (normal distribution)				Beta Distribution	
		Low	High	Mean	Std Deviation		Upper Limit	Lower Limit	Mean	Std Deviation	A	B
Sat. Moist. Content (θ_s)[*][3]	48	0.321	0.566	0.438	0.059	NO	-	-	-	-	-	-
Res. Moist. Content (θ_r)[*]	48	0.016	0.11	0.062	0.027	SN	0	0.881	0.458	0.255	-	-
Res. Saturation (S)[**]	50	0.020	0.399	0.159	0.0816	BETA					3.0234	16.0225
Van Genuchten α (1/cm)	48	0.0008	0.387	0.034	0.072	LN	-7.131	-0.949	-4.489	1.352	-	-
Van Genuchten n	48	1.262	2.894	1.824	0.344	NO	-	-	-	-	-	-
Sat. Conductivity (K_s)(cm/s)	40	5.80E-06	1.70E-02	1.00E-03	3.00E-03	LN	-12.058	-4.057	-8.487	1.813	-	-
Longitudinal Dispersivity (m)	NA	0.0279	0.0341	0.031	NA	UN	-	-	-	-	-	-
Bulk Density[2]	NA	-	-	1.65	-	CO	-	-	-	-	-	-

Ringold gravel (I.e. fluvial unit E) - based on Khaleel and Freeman (1995) soil category SG2 (sandy gravel with gravel fraction >60%)

Parameter	Number of samples	Raw				Transform	Transformed (normal distribution)				Beta Distribution	
		Low	High	Mean	Std Deviation		Upper Limit	Lower Limit	Mean	Std Deviation	A	B
Sat. Moist. Content (θ_s)[*][3]	11	0.056	0.107	0.077	0.016	LN	-2.88	-2.234	-2.59	0.216	-	-
Res. Moist. Content (θ_r)[*]	11	0	0.0197	0.01	0.007	NO	-	-	-	-	-	-
Res. Saturation (S)[**]	11	0	0.229	0.143	0.0807	BETA					2.5566	15.2920
Van Genuchten α (1/cm)	11	0.003	0.028	0.009	0.009	LN	-5.952	-3.59	-5.008	0.882	-	-
Van Genuchten n	11	1.347	1.885	1.621	0.178	NO	-	-	-	-	-	-
Sat. Conductivity (K_s)(cm/s)	10	2.83E-05	1.30E-01	1.40E-02	4.10E-02	LN	-10.473	-2.04	-7.137	2.332	-	-
Longitudinal Dispersivity (m)	NA	0.027	0.178	0.09	NA	UN	-	-	-	-	-	-
Bulk Density[2]	NA	-	-	2.07	-	CO	-	-	-	-	-	-

[*] After Khaleel and Freeman (1995).
[**] Calculated by dividing the θ_r by the θ_s raw data presented in Khaleel and Freeman (1995)
[†] NO = Normal (no transformation required); LN = Lognormal; LR = Log ratio; SN = Hyperbolic arcsine; UN = Uniform, CO = Constant
[1] Taken from Ho, et. al., 1999 [Stochastic Parameter Development for PORFLOW Simulations of the Hanford AX Tank Farm].
[2] Taken from Khaleel, et. al. 2000 (Modeling Data Package for S-SX Field Investigation Report (FIR)).
[3] Values for effective porosity are assumed to be equal to the saturated water content.
[4] This is a 4-parameter distribution, where two of the parameters are the minimum and maximum value. The other two parameters are represented here

Kincaid et al. (1998) defined several K_d classes for mapping distribution coefficients to high or intermediate impact zones and chemical waste type. These K_d classes were labeled A through H (Table 4.9). To account for the common observation that significant gravel content decreases K_d values (Kaplan and Serne 1999), the intermediate impact zone for each K_d class in the SAC Rev. 0 initial assessment was further subdivided into gravel rich and gravel poor zones. K_d classes containing a "1" pertain to gravel poor (i.e. sand) strata and K_d classes containing a "2" pertain to gravel rich (gravelly sand and sandy gravel) strata (Table 4.9). In accordance with the gravel corrections applied by Kaplan and Serne (1999), all K_d values assigned to the gravel rich hydrogeologic units were decreased by an order of magnitude from those assigned to the sand rich units, see Attachment 3.[3] Attachment 1 identifies the K_d classes assigned to each hydrostratigraphic unit for each aggregate area. As with the hydraulic parameters, all model nodes within a single hydrogeologic unit are assigned the same K_ds for a single realization.

4.2   Site-Specific Templates

Of the more than 1200 waste sites at Hanford, a subset of 890 sites was selected for inclusion in the initial assessment (See *Appendix A - Inventory Data for Initial Assessment Performed with the System Assessment Capability (Revision 0))*. Six hundred eighty-nine of these sites, mostly planned (intentional) liquid discharge sites, will be simulated individually. The remained 201 dry waste burial grounds and unplanned releases have been aggregated into 30 aggregate sites based on their location, waste release model, and waste chemistry designations. This effectively reduced the number of sites to be simulated and thus aids computational efficiency. The combination of individual liquid discharge sites and the aggregated burial ground and unplanned release sites brought the total number of sites to be simulated down, from 890 to 719 (See Attachment 2).

Each vadose zone site (whether it represents a single Hanford facility or an aggregation of several) is identified by a unique alphanumeric identification tag. In the case of single sites simulated without aggregation it was desirable that the site ID be transparent, that is, that it be represented using the site code as given in the Hanford WIDS system. For example, the 216-T-106 tank is identified by its WIDS site code "216-T-106". For multiple sites simulated as an aggregated site, it was desirable that as much of the WIDS system site code as the sites have in common be used, and then some information suggestive of the aggregation be included. Thus, a dollar sign is used to delimit between the "real" portion (using as much of the WIDS code as all the sites to be aggregated have in common) and the base template code (which denotes the geography, facility type, and waste category that the aggregated sites have in common). The dollar sign ($) is followed by the letter designating the geographic area of the base template used and a number (1 to 6) designating the waste chemistry type, followed by a dash (-) and the number of actual sites represented by this aggregation. For example, there are 11 dry-waste burial grounds within the northern portion of 200 East Area (Aggregate Area "B"), which are all designated as waste type 6 with a soil/debris release model. These sites were all aggregated together and assigned the designation 218-E$B6-11.

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[3] Letter Report to George Last from Kenneth Krupka. September 29, 2000. Subject: K_d Values for Composite Analysis. (Attachment 3)

Table 4.9. Distribution of K_ds by Waste Chemistry Designation

Waste Chemistry/Source Category 1: High Organic/Very Acidic

Element	High Impact (A) Best Kd Estimate (mL/g)	High Impact (A) Range Kd Estimate (mL/g)	Intermediate Impact - Sand (B1) Best Kd Estimate (mL/g)	Intermediate Impact - Sand (B1) Range Kd Estimate (mL/g)	Intermediate Impact - Gravel (B2) Best Kd Estimate (mL/g)	Intermediate Impact - Gravel (B2) Range Kd Estimate (mL/g)	Groundwater (F1) Best Kd Estimate (mL/g)	Groundwater (F1) Range Kd Estimate (mL/g)	Probability Distribution
Tritium	0	0	0	0	0	0	0	0	NA
Technetium	0	0	0	0	0	0	0	0	NA
Iodine	0	0	0.1	0 to 1	0.01	0 to 0.1	0.5	0 to 15	log normal*
Uranium	0.2	0.1 to 1	0.2	0.2 to 10	0.02	0.02 to 1.0	3	0.1 to 500	log normal*
Strontium	0.4	0.1 to 5	7	5 to 20	0.7	0.5 to 2.0	20	0.2 to 173	log normal*
Cesium	0.3	0 to 2	20	20 to >200	2	2.0 to >20.0	300	40 to 2000	log normal*
Plutonium	0.4	0.1 to 1	25	15 to 50	2.5	1.5 to 5.0	200	80 to >1980	log normal*
Carbon Tetrachloride	0.192	0 to 1.3	0.192	0 to 1.3	0.02	0 to 0.13	0.2	0.1 to 0.6	log normal*
Chromium (VI)	0	0	0	0	0	0	0	0	NA

Waste Chemistry/Source Category 2: High Organic/Near Neutral

Element	High Impact (B1) Best Kd Estimate (mL/g)	High Impact (B1) Range Kd Estimate (mL/g)	Intermediate Impact - Sand (B1) Best Kd Estimate (mL/g)	Intermediate Impact - Sand (B1) Range Kd Estimate (mL/g)	Intermediate Impact - Gravel (B2) Best Kd Estimate (mL/g)	Intermediate Impact - Gravel (B2) Range Kd Estimate (mL/g)	Groundwater (F1) Best Kd Estimate (mL/g)	Groundwater (F1) Range Kd Estimate (mL/g)	Probability Distribution
Tritium	0	0	0	0	0	0	0	0	NA
Technetium	0	0	0	0	0	0	0	0	NA
Iodine	0.1	0 to 1	0.1	0 to 1	0.01	0 to 0.1	0.5	0 to 15	log normal*
Uranium	0.2	0.2 to 10	0.2	0.2 to 10	0.02	0.02 to 1.0	3	0.1 to 500	log normal*
Strontium	7	5 to 20	7	5 to 20	0.7	0.5 to 2.0	20	0.2 to 173	log normal*
Cesium	20	20 to >200	20	20 to >200	2	2.0 to >20.0	300	40 to 2000	log normal*
Plutonium	25	15 to 50	25	15 to 50	2.5	1.5 to 5.0	200	80 to >1980	log normal*
Carbon Tetrachloride	0.192	0 to 1.3	0.192	0 to 1.3	0.02	0 to 0.13	0.2	0.1 to 0.6	log normal*
Chromium (VI)	0	0	0	0	0	0	0	0	NA

Waste Chemistry/Source Category 3: Very High Salt/Very Basic

Element	High Impact (D) Best Kd Estimate (mL/g)	High Impact (D) Range Kd Estimate (mL/g)	Intermediate Impact - Sand (E1) Best Kd Estimate (mL/g)	Intermediate Impact - Sand (E1) Range Kd Estimate (mL/g)	Intermediate Impact - Gravel (E2) Best Kd Estimate (mL/g)	Intermediate Impact - Gravel (E2) Range Kd Estimate (mL/g)	Groundwater (F1) Best Kd Estimate (mL/g)	Groundwater (F1) Range Kd Estimate (mL/g)	Probability Distribution
Tritium	0	0	0	0	0	0	0	0	NA
Technetium	0	0	0	0	0	0	0	0	NA
Iodine	0	0 to 1.1	0	0 to 2	0	0 to 0.2	0.5	0 to 15	log normal*
Uranium	20	10 to 800	0.3	0 to 3	0.03	0 to 0.3	3	0.1 to 500	log normal*
Strontium	10	4 to 20	0.5	0.3 to 42	0.05	0.03 to 4.2	20	0.2 to 173	log normal*
Cesium	1.5	1 to 25	500	64 to 1360	50	6.4 to 136.0	300	40 to 2000	log normal*
Plutonium	10	5 to 100	20	5 to >98	2	0.5 to >9.8	200	80 to >1980	log normal*
Carbon Tetrachloride	0.192	0 to 1.3	0.192	0 to 1.3	0.02	0 to 0.13	0.2	0.1 to 0.6	log normal*
Chromium (VI)	0	0	0	0	0	0	0	0	NA

Waste Chemistry/Source Category 4: Chelates/High Salts

Element	High Impact (G1) Best Kd Estimate (mL/g)	High Impact (G1) Range Kd Estimate (mL/g)	Intermediate Impact - Sand (G1) Best Kd Estimate (mL/g)	Intermediate Impact - Sand (G1) Range Kd Estimate (mL/g)	Intermediate Impact - Gravel (G2) Best Kd Estimate (mL/g)	Intermediate Impact - Gravel (G2) Range Kd Estimate (mL/g)	Groundwater (C) Best Kd Estimate (mL/g)	Groundwater (C) Range Kd Estimate (mL/g)	Probability Distribution
Tritium	0	0	0	0	0	0	0	0	NA
Technetium	0	0	0	0	0	0	0	0	NA
Iodine	0	0 to 0.5	0	0 to 0.5	0	0 to 0.05	0.5	0.2 to 15	log normal*
Uranium	0.4	0.2 to 3	0.4	0.2 to 3	0.04	0.02 to 0.3	3	0.1 to 79.3	log normal*
Strontium	5	0 to 30	5	0 to 30	0.5	0 to 3.0	4	2 to 20	log normal*
Cesium	10	6 to 18	10	6 to 18	1	0.6 to 1.8	300	67 to 1330	log normal*
Plutonium	3	0.6 to 100	3	0.6 to 100	0.3	0.06 to 10.0	40	20 to >1980	log normal*
Carbon Tetrachloride	0.192	0 to 1.3	0.192	0 to 1.3	0.02	0 to 0.13	0.2	0.1 to 0.6	log normal*
Chromium (VI)	0	0	0	0	0	0	0	0	NA

Waste Chemistry/Source Category 5: Low Organic/Low Salts/Acidic

Element	High Impact (H) Best Kd Estimate (mL/g)	High Impact (H) Range Kd Estimate (mL/g)	Intermediate Impact - Sand (F1) Best Kd Estimate (mL/g)	Intermediate Impact - Sand (F1) Range Kd Estimate (mL/g)	Intermediate Impact - Gravel (F2) Best Kd Estimate (mL/g)	Intermediate Impact - Gravel (F2) Range Kd Estimate (mL/g)	Groundwater (F1) Best Kd Estimate (mL/g)	Groundwater (F1) Range Kd Estimate (mL/g)	Probability Distribution
Tritium	0	0	0	0	0	0	0	0	NA
Technetium	0.2	0	0	0	0	0	0	0	NA
Iodine	0.2	0.1 to 2	0.5	0 to 15	0.05	0 to 1.5	0.5	0 to 15	log normal*
Uranium	30	20 to 200	3	0.1 to 500	0.3	0.01 to 50	3	0.1 to 500	log normal*
Strontium	50	50 to 200	20	0.2 to 173	2	0.02 to 17.3	20	0.2 to 173	log normal*
Cesium	30	10 to 100	300	40 to 2000	30	4.0 to 200	300	40 to 2000	log normal*
Plutonium	50	20 to 200	200	80 to >1980	20	8.0 to >198.0	200	80 to >1980	log normal*
Carbon Tetrachloride	0.192	0 to 1.3	0.192	0 to 1.3	0.02	0 to 0.13	0.2	0.1 to 0.6	log normal*
Chromium (VI)	0	0	0	0	0	0	0	0	NA

Waste Chemistry/Source Category 6: Low Organic/Low Salt/Near Neutral

Element	High Impact (F1) Best Kd Estimate (mL/g)	High Impact (F1) Range Kd Estimate (mL/g)	Intermediate Impact - Sand (F1) Best Kd Estimate (mL/g)	Intermediate Impact - Sand (F1) Range Kd Estimate (mL/g)	Intermediate Impact - Gravel (F2) Best Kd Estimate (mL/g)	Intermediate Impact - Gravel (F2) Range Kd Estimate (mL/g)	Groundwater (F1) Best Kd Estimate (mL/g)	Groundwater (F1) Range Kd Estimate (mL/g)	Probability Distribution
Tritium	0	0	0	0	0	0	0	0	NA
Technetium	0	0	0	0	0	0	0	0	NA
Iodine	0.5	0 to 15	0.5	0 to 15	0.05	0 to 1.5	0.5	0 to 15	log normal*
Uranium	3	0.1 to 500	3	0.1 to 500	0.3	0.01 to 50	3	0.1 to 500	log normal*
Strontium	20	0.2 to 173	20	0.2 to 173	2	0.02 to 17.3	20	0.2 to 173	log normal*
Cesium	300	40 to 2000	300	40 to 2000	30	4.0 to 200	300	40 to 2000	log normal*
Plutonium	200	80 to >1980	200	80 to >1980	20	8.0 to >198.0	200	80 to >1980	log normal*
Carbon Tetrachloride	0.192	0 to 1.3	0.192	0 to 1.3	0.02	0 to 0.13	0.2	0.1 to 0.6	log normal*
Chromium (VI)	0	0	0	0	0	0	0	0	NA

Taken from the Composite Analysis (Kincaid et. al., 1998)
Taken from Last and Rohay (1993)
After Ken Krupka's Review, Sept. 2000 (Attachment 3)
After Ken Krupka's Review, Sept. 2000, considering range Kd estimate values in ILAW-PA data package (Attachment 3)
After Cantrell's White Paper, Aug. 2000 (Attachment 3) and Ken Krupka's review, Sept. 2000 (Attachment 3)
Defined by "Best Estimate" (as median) with minimum as lower bound (After Letter Report by Last and Cantrell (2001) (Attachment 3)).

Initially each site (or aggregate site) was assigned to a base template based on its location within one of the 13 aggregate areas, its site type (surface, near surface, tank, or injection well), and its waste chemistry designation. Once the base template was identified, other site-specific template information (location, area, and recharge rates) was developed.

4.2.1 Assignment of Waste Types

Wherever possible, the same waste chemistry designations used in the Composite Analysis (Kincaid et al. 1998) were also assigned to the facilities and unplanned releases designated for simulation in the initial assessment. However, for facilities not included in the Composite Analysis, the following approach was taken.

- Burial grounds, process sewers, ponds, retention basins, buildings, cooling water, stacks, steam condensate, and sand filters were assigned a "low organic, low salt, near neutral" waste type (waste type 6).
- All 241 facilities were assigned a "high ionic strength, very basic" waste type (waste type 3). Note that some tank wastes are designated as containing chelates and high salt (waste type 3) (Kincaid et al. 1998). This simplifying assumption to group essentially all tank waste into just two waste types on which to assign Kd values does have obvious limitations.
- Liquid waste facilities that still lacked a waste type, were assigned a waste type based on waste descriptions by Maxfield (1979) and/or the various Source Aggregate Area Management Study Reports (e.g. DOE 1992; DOE 1993c)
- The WIDS was consulted for all remaining facilities. If the WIDS indicated a source for the effluent discharged to a facility, the facility was given the waste type for the source. In a few instances, WIDS provided no information and a waste type 6 was assigned.
- Unplanned releases associated with a facility were assigned the waste type given to the facility.
- Unplanned releases of solids (e.g. animal waste, contaminated equipment, particulates), and atmospheric releases were assigned waste type 6.
- Unplanned releases with insufficient information were assigned a best guess of waste type 6.
- Petroleum spills are obviously high organic but they do not fit the idea of Z Plant waste types 1 and 2. Therefore, petroleum spills were arbitrarily labeled waste type 6.

The waste chemistry designations for all facilities represented in the initial assessment are provided in Attachment 2. Note that only sites with the same waste designation have been aggregated together.

4.2.2 Facility Location, Area, and Wetted Column Area

The location and surface area for most waste facilities were obtained from the WIDS. Facility locations are assumed to be the center of the facilities (in state-plane coordinates). The area, or footprint, of each facility was taken from WIDs where available, or calculated as a function of the facility length and width, or facility diameter (where such information was available). It is assumed that these data represent the actual footprint of the area, however, there is some indication that these data may represent the fenced boundaries of the radiation zone surrounding the facility. If so, this may result in a larger wetted column area than the actual foot print would suggest, and would cause a slower rate of downward migration.

For those facilities where locations and/or dimensions were not provided by WIDS the missing data were estimated using other available resources such as the *Hanford Site Waste Management Units Report*[3], the *Hanford Site Atlas* (BHI 1998) and Maxfield (1979). Long linear facilities

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[3] http://www.bhi-erc.com/eis/wids/hswmuri.pdf

(such as ditches) generally do not have center coordinates listed in WIDS, so their coordinates were estimated based on visual inspection of the *Hanford Site Atlas* and/or other site maps.

The locations of aggregated sites (i.e. the combination of more than one site) were determined by averaging the centroid coordinates for each of the individual sites included in the aggregation. Their footprint areas were determined by summing all of the site areas for each individual site included in the aggregated site. Attachment 2 provides all available facility locations and footprint areas.

Generally speaking, the wetted column area for SAC Rev. 0 simulations are assumed to be equal to the footprint area of the facility. For example, the wetted column area beneath the high level waste tanks (e.g. 241-T-106) is assumed to be the area of the tank bottom. However, for high volume liquid disposal sites (i.e. those with an average annual infiltration rate >20 m^3/m^2 [like 216-A-8]) a 2x area multiplier was used to increase the wetted column areas to account for lateral spreading, better simulate actual contaminant distributions, and facilitate numerical solution of the simulations. This is a similar approach to that used in the Composite Analysis (Kincaid, et. al. 1998), where they used a value of three times the area necessary to pass the crib discharges through the strata with the lowest saturated conductivity without ponding. However, unlike the Composite Analysis, the stochastic approach and simplified design for SAC Rev. 0 limits the Vadose Zone column to a constant area independent of the hydraulic properties. Initial tests with input values drawn near the lower bounds of the stochastic distributions, resulted in cases of fully saturated, overpressurized vadose zone columns, that failed to reach a numerical solution, and that would not reflect the physical reality. Therefore, after some trial and error along with professional judgement, the 2x area multiplier was selected for the higher volume liquid discharge sites.

For reverse wells, the wetted column area was determined by calculating the pore volume that would be fully saturated by the average annual discharge volume, and then dividing this by the facility area. For example:

> The 216-B-5 reverse well was perforated from 74 to 92 m below ground surface (Smith, 1980). The entire perforated interval is within a Hanford formation sand sequence that extends to 25 m below the bottom of 216-B-5. Typical saturated volumetric water content (porosity) for Hanford formation sand is between 33 and 49 vol. % (excluding the highest and lowest values; Connelly et al., 1992). A middle value of 40-vol. % was used for the estimate. An estimated average annual discharge to 216-B-5 (calculated by dividing the total discharge volume by the number of years the facility operated) is 15,300 m^3. Using these data the saturated pore volume is:
>
> Saturated pore volume (m^3) = (15,300 m^3 Ave. ann. discharge) / (0.4 porosity) = 38,250 m^3.
>
> Assuming that the saturated pore volume is a cube, then area of the soil column is $(38,250 \text{ m}^3)^{2/3} = 1135 \text{ m}^2$. Dividing this by the facility area (0.033 m^2) yields the area multiplier (34401). (Note, this may seem like a very large multiplier, but the bottom area of a reverse well is the based on the diameter of the well casing, in this case 20 cm [8 inches.])

Those sites for which a facility area could not be found, measured, calculated, or even guessed at, were assigned a default value. These default values were all based on some combination of three "9"s for easy recognition as a default value. Table 4.10 lists the default values used for different site types.

Table 4.10. Default Areas

Facility (Site) Type	Default Area (m^2)
Unplanned Release, French Drain	0.999
Storage Tank, Trench	9.99
Radioactive Process Sewer, Crib	99.9
Burial Ground	999

4.3   Recharge Estimates

SAC Rev. 0 incorporates recharge estimates into the STOMP model as deterministic values that change stepwise as the surface cover changes, and change as linear function of time to represent the degradation of engineered covers following their design life. The recharge rates (actually, deep drainage rates) used for SAC Rev. 0 were estimated for all surface conditions under consideration for the initial assessment. These conditions include four different barrier designs, degraded barriers, the natural conditions that surround the barriers, and the unique conditions created by human activities (e.g., facility construction; gravel-covered tank farms). Recharge estimates were based on the best available data (Fayer and Walters 1995; Fayer, et. al., 1999; Murphy et. al., 1996; Prych, 1998)

4.3.1 Barrier Recharge Estimates

Recharge through engineered surface covers was estimated based on the focused feasibility study (FFS) conducted by the Department of Energy (DOE/RL 1996). The FFS was conducted to determine the barrier needs at Hanford and identify a set of barrier designs to meet those needs. Table 4.11 identifies the four barrier designs that were proposed (DOE/RL 1996). According to the FFS, the Modified RCRA C design will be the predominant barrier type. DOE/RL (1996) used the Hydrologic Evaluation of Landfill Performance (HELP) model to simulate the recharge rate through the Hanford Barrier and the modified RCRA barriers. The estimates ranged from 0.2 to 0.8 mm/yr., assuming that the annual mean precipitation remained at 160 mm/yr. Subsequent to the FFS, additional data and model results became available. As a result the recharge rates for the barriers were updated and are reflected in Table 4.11.

Table 4.11. Barrier design lifetimes and estimated recharge rates (actual rates are expected to be less than shown).

DOE/RL Design	Design Life (yr.)	Recharge Rate (mm/yr.)	Source
Hanford Barrier	1000	0.1	Based on lysimeter data and simulation results (Fayer et al. 1999)
Modified RCRA C	500	0.1	Based on lysimeter data and simulation results (Fayer et al. 1999)
Standard RCRA C	30	0.1	No data; recommendation is based on presence of geomembrane, 2-ft thick clay admix layer, and short design life
Modified RCRA D	100	0.1	Based on simulation results using parameters from Fayer et al. (1999)

No guidance is available for specifying barrier performance after the design life. However, we do not expect an immediate decrease in performance and it's very possible that some of these

barriers will perform as designed far beyond their design life. Without data to understand and predict that long-term performance, however, we assumed that the performance would decrease linearly after reaching its design life, until the recharge rate matches the rate in the surrounding environment. This approach is based on the assumption that a degraded cover will behave like the surrounding environment. We also assumed that the period of degradation would be the same as the design life. For example, the modified RCRA D cover performs as designed for 100 years, then degrades linearly over the next 100 years to the point where recharge rates are equivalent to the rates of the natural surrounding environment.

The schedule and type of engineered cover to be applied to each site (Attachment 2) was based on the Hanford Disposition Baseline as defined in the *System Assessment Capability (Revision 0) Assessment Description, Requirements, Software Design and Test Plan*[1], and subsequent information supplied by 200 Area Remediation Project staff[2].

4.3.2 Natural (non-barrier) Recharge Rates

Most of the Hanford Site, including some innocuous waste sites, have not had and will not have a surface barrier. The estimated recharge in these areas addressed four site conditions:

- undisturbed soil and shrub-steppe (a plant community consisting of shrubs and bunchgrasses and associated fauna and flora),
- undisturbed soil with no vegetation (e.g., Hanford operations),
- disturbed soil with no vegetation (e.g., Hanford sand exposed during operations; gravel-covered soil), and
- disturbed soil with shrub-steppe (e.g., Hanford sand exposed during operations but subsequently re-vegetated).

The Hanford soil map (Hajek 1966) was examined to identify the soil types prevalent in the waste areas. Table 4.12 lists the four soil types that dominate the areas being evaluated in the initial assessment and their recharge rates. Our assumption is that these soils, in their undisturbed condition, support a shrub-steppe plant community.

During Hanford operations, the shrub-steppe plant community was often removed while leaving the existing soil type relatively intact. In other areas, the sites were excavated, which removed the existing soil structure and replaced it with backfilled Hanford-formation sand or gravel. Operations also covered selected surface areas with a layer of gravel (e.g., tank farms). Table 4.13 shows the estimated recharge rates for native soils and backfilled sediments without vegetation. Eventually, the disturbed areas may become re-vegetated and a shrub-steppe plant community re-established. Thus, the estimated recharge rate is assumed to return to that equivalent to the pre-Hanford conditions.

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[1] These documents can be found at http://www.bhi-erc.com/vadose/sac.htm#info
[2] Contact Bruce Ford, Bechtel Hanford Incorporated.

Table 4.12. Estimated recharge rates for predominant soil types and sediments with a shrub-step plant community.

Soil Type	Recharge Rate Estimate (mm/yr.)	Description
Ephrata stony loam (E_b)	1.5	No data; used estimate for E_l, which is a similar soil
Ephrata sandy loam (E_l)	1.5	Avg. of two estimates (1.2; 1.8) from deep (> 10 m) chloride data collected from the two boreholes B17 and B18 (Prych 1998)
Burbank loamy sand (B_a)	3.0	Avg. of three estimates (0.66, 2.8, 5.5) from deep (> 10 m) chloride data collected from the three boreholes B10, B12, and B20 (Prych 1998)
Rupert Sand (R_p) in 200 East	0.9	Avg. of four estimates (0.16, 0.58, 1.0, and 1.8) from deep (> 10 m) chloride data collected from the four boreholes E24-161, E24-162, B8501, B8502 (Fayer et al. 1999)
Rupert Sand (R_p) outside of 200 East	4.0	Estimated from chloride data collected from a borehole near the Wye Barricade (Murphy et al. 1996)
Hanford-formation sand	4.0	No data; used estimate for Rupert sand outside the 200 East area

Table 4.13. Estimated recharge rates for native soils and backfilled sediments without vegetation.

Soil Type	Recharge Rate Estimate (mm/yr.)	Description
Ephrata stony loam (E_b)	17.3	Simulation estimate from Fayer and Walters (1995)
Ephrata sandy loam (E_l)	17.3	Simulation estimate from Fayer and Walters (1995)
Burbank loamy sand (B_a)	52.5	Simulation estimate from Fayer et al. (1999)
Rupert Sand (R_p)	44.3	Simulation estimate from Fayer et al. (1999)
Hanford-formation sand	55.4	8-yr lysimeter record for Hanford sand (Fayer and Walters 1995)
Graveled surface	104	8-yr lysimeter record for graveled surface (Fayer et al. 1999)

4.3.3 Summary of recharge estimates for the initial assessment

The estimated recharge rates for various surface conditions for each of the 13 aggregate areas is provided in Table 4.14. This table presents a brief description of each setting and identifies the major soil type that was identified visually for each area using the Hajek (1966) soil map. If a significant secondary soil type was present, that soil type is shown in parentheses. Likewise, its recharge rate is also shown in parentheses.

The recharge rates estimated for the initial assessment do not account for overland flow from roadways or roofs, water line leaks, or any other anthropogenic additions of water. The rates also do not account for variations within soil types, plant community succession (e.g., a takeover by cheatgrass), dune sand deposition, or climate change. Finally, these rates were developed for fairly large geographic areas and may not represent the local recharge rates at specific locations.

Table 4.14. Recharge estimates for the initial assessment. Significant secondary soil types and their associated recharge estimates are shown in parentheses.

Area Label	Brief Description	Major (Secondary) [1] Soil Type(s)	Recommended Recharge Rate (mm/yr.)			
			Pre- and Post-Hanford (shrub-steppe)	Operations (soil intact, no vegetation)	Operations (soil disturbed, with/without vegetation)	Operations (gravel surface, no vegetation)
C	Reactor along river	E_b (B_a)	1.5 (3.0)	17.3 (52.5)	4.0 / 55.4	104
K	Reactor along river	E_b (E_l)	1.5 (1.5)	17.3 (17.3)	4.0 / 55.4	104
N	Reactor along river	E_b	1.5	17.3	4.0 / 55.4	104
D	Reactor along river	E_l	1.5	17.3	4.0 / 55.4	104
H	Reactor along river	B_a	3.0	52.5	4.0 / 55.4	104
F	Reactor along river	R_p (E_l)	4.0 (1.5)	44.3 (17.3)	4.0 / 55.4	104
R	300 Area	R_p (E_l)	4.0 (1.5)	44.3 (17.3)	4.0 / 55.4	104
G	200N Area	E_l (B_a)	1.5 (3.0)	17.3 (52.5)	4.0 / 55.4	104
T	Northern 200W Area	R_p (B_a)	4.0 (3.0)	44.3 (52.5)	4.0 / 55.4	104
S	Southern 200W Area and ERDF	R_p	4.0	44.3	4.0 / 55.4	104
A	Southern 200E Area	R_p (B_a)	0.9 (3.0)	44.3 (52.5)	4.0 / 55.4	104
B	Northwestern 200E Area	E_l	1.5	17.3	4.0 / 55.4	104
E	Eastern 200E Area	B_a (R_p)	3.0 (0.9)	52.5 (44.3)	4.0 / 55.4	104

E_b = Ephrata stony loam E_l = Ephrata sandy loam B_a = Burbank loamy sand R_p = Rupert sand
[1] Note: Only the major soil types were used to represent each aggregate area.

5.0   Summary

The initial (proof of principal) assessment conducted using the System Assessment Capability (SAC Rev. 0) includes one-dimensional stochastic simulations of flow and transport through the vadose zone. Data and interpreted information needed to define the input parameters for the STOMP code were extracted from existing documents and databases. Eight hundred ninety waste sites have been selected for simulation, either as individual liquid discharge sites or included in aggregated burial ground or unplanned release sites. Burial ground and unplanned release sites were aggregated together based on their location, waste release model, and waste chemistry designations.

To simplify the preparation of input files for the large number of sites, and to improve the computational efficiencies, the Hanford Site was subdivided into 13 geographically similar areas that could be represented by a single generalized hydrogeologic column. The hydrogeologic columns for each of the 13 aggregate areas were further modified to account for differences in the depth of waste releases, and differences in solid/liquid distribution coefficients (K_ds) effected by different waste chemistries. This resulted in 64 base templates, each with their own unique hydrogeologic stratigraphy, hydraulic parameter distributions, and K_d distributions. Stochastic parameters are sampled for each hydrogeologic unit for each realization. Thus, each node with in given hydrogeologic unit has the same set of parameters for a given realization.

This report describes the assumptions and rationale for 1) defining the hydrostratigraphy, hydraulic properties, and distribution coefficients for each base template; 2) defining which base template to be assigned to each site to be simulated, and 3) defining the site location, footprint area, wetted column area, and recharge estimates for each site.

6.0   References

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Attachment 1
Base Hydrostratigraphic Templates

Attachment 2
SAC Rev. 0 Site List and Template Designations

Attachment 3
Reviews of K$_d$ Values for SAC Rev. 0

Includes:

A) White Paper by Kirk Cantrell, August 2, 2000, Estimation of Carbon Tetrachloride Adsorption Coefficient for Hanford Sediments.

B) Letter Report by Kenneth Krupka to George Last, September 29, 2000, K$_d$ Values for Composite Analysis.

C) Letter Report by George Land and Kirk Cantrell to Distribution, January 4, 2001, Kd Distributions for SAC Rev. 0.

Estimation of the Carbon Tetrachloride Adsorption Coefficient
for Hanford Sediments

Kirk Cantrell, 8/2/00

The mobility of nonionic organic chemicals in natural aquifer systems is largely controlled by their solubility in water and affinity for aquifer solids. The relative affinity that a particular nonionic organic compound has for a specific soil or sediment can be described mechanistically as hydrophobic adsorption (Westall, 1987). Hydrophobic adsorption is driven by the incompatibility of the nonpolar compounds with water. As a result, it is possible to characterize the adsorption of a wide range of organic compounds on a wide range of sorbents based on a single property of the compound (e.g., its octanol-water partition constant, K_{ow}) and a property of the sorbent (the fraction of the sorbent that is organic carbon, f_{oc})(Karickhoff, 1984; Karickhoff et al., 1979; Schwarzenbach and Westall, 1981). Efforts to model the sorption of nonionic organic substances using octanol/water partition coefficients have proven to be reasonably successful (Karickhoff, 1981), but can be problematic. Voice and Weber (1985) suggested that K_{ow} values may tend to underpredict the partitioning of hydrophobic compounds between water and particulate organic carbon because of mutual saturation effects. Moreover, experimental determinations of K_{ow} are time consuming, and may lack analytical precision and accuracy (Chin et al., 1988)

A number of investigators have observed that the sorption of uncharged hydrophobic organic compounds can be correlated to the organic carbon content of the sorbent (Lambert et al., 1965; Karickhoff et al., 1979; Means et al., 1980; Brownawell and Farrington, 1986). For such cases partition coefficient values (or distribution coefficients, K_d) can be normalized in terms of the fraction of organic carbon (f_{oc}) associated with the sorbent to yield an organic-carbon-partition coefficient, K_{oc}.

$$K_{oc} = K_d/f_{oc} \qquad (1)$$

Karickhoff et al. (1979) observed a generally good relationship between K_d and K_{oc}, but noted the occurrence of deviations for sandy soils having low organic carbon content ($f_{oc} < 0.001$).

Organic carbon content analyses that are available for Hanford Site Sediments are tabulated in Appendix 1. Note that although a few analyses contain organic carbon fractions above 0.001, both the average (0.00094) and the median (0.00030) are below the values where equation 1 appears to be generally applicable.

K_{oc} values for carbon tetrachloride were estimated by Truex (2000) using two different approaches. These two methods resulted in values of 110 ml/gm and 161 ml/gm. Taking the average of these values (136 ml/gm) and the average f_{oc} of 0.00094, a K_d value of 0.13 ml/gm is calculated. Although this value could be used in the absence of any alternatives, it is possible that this value could underestimate the actual degree of carbon tetrachloride adsorption to Hanford Sediments. At the very low organic carbon contents observed for Hanford Sediments adsorption onto mineral surfaces could become more significant than adsorption due to the organic matter alone.

Another method for estimating K_d values for carbon tetrachloride for Hanford sediments can be used as an alternative to using equation 1 and estimated K_{oc} values and measured values

of f_{oc}. For this alternative, K_d values for carbon tetrachloride are estimated using measured values measured for low organic content sediments that are sandy in character like Hanford sediments. Because adsorption of carbon tetrachloride is through a hydrophobic mechanism, differences in specific mineralogy between these sediments and Hanford sediments is likely to have a minor affect on the K_d values. In this case, the texture or surface area of the sediment is likely to have a much greater impact on the adsorption than the mineralogy.

Brusseau et al. (1991) measured retardation factors for carbon tetrachloride in an aquifer material that was greater than 98% sand (Rabis baek). The fraction of organic carbon for this material was 0.00007. Using the given bulk density and pore water content a K_d of 0.25 ml/gm was calculated (for 10°C).

A series of field and laboratory investigations were conducted at a site in Borden, Ontario to evaluate the transport of a halogenated hydrocarbon compounds (Makay et al., 1986; Roberts et al., 1986; Curtis et al, 1986). The Borden aquifer material is a clean, well-sorted, fine- to medium grained sand with an average organic carbon fraction of 0.0002 (range 0.0001 to 0.0009) (Mackay et al., 1986). Batch experiments conducted at 21°C resulted in a K_d of 0.15 ml/gm. After correcting for differences in temperature, retardation factors calculated with this K_d value were in very good agreement with retardation factors determined from both temporal and spatial field data.

Chin et al. (1988) measured a K_d value for a soil collected from Michawye Michigan. This soil had a sandy character and a fractional organic carbon content of 0.0013. The K_d value was determined to be 0.542 ml/gm (presumably at room temperature).

Based on the data presented here it is estimated that the most probable value for a K_d for carbon tetrachloride adsorption onto Hanford sediment is 0.2 ml/gm, with a range of approximately 0.1 to 0.6.

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Appendix 1. Hanford Sediment Organic Carbon Values.

Well or Sample Number	Depth, ft	Fraction Organic Carbon	Reference
299-W11-30	67.1	0.00055	Newcomer et al., 1995
299-W11-30	70.1	0.00041	Newcomer et al., 1995
299-W11-30	82.9	0.00005	Newcomer et al., 1995
299-W11-30	85.3	0.00515	Newcomer et al., 1995
299-W11-32	74.4	0.00005	Newcomer et al., 1995
299-W11-32	77.1	0.00016	Newcomer et al., 1995
299-W11-32	83.5	0.00019	Newcomer et al., 1995
299-W11-32	89	0.00022	Newcomer et al., 1995
299-W11-32	93	0.00076	Newcomer et al., 1995
299-E28-26	39-40	0.0006	Ames and Serne, 1991
299-E28-26	129-130	0.0021	Ames and Serne, 1991
299-E28-26	129-130	0.0000	Ames and Serne, 1991
299-E28-26	294-295	0.0000	Ames and Serne, 1991
299-E28-26	319-320	0.0001	Ames and Serne, 1991
299-E33-30	39-40	0.0002	Ames and Serne, 1991
299-E33-30	139-140	0.0005	Ames and Serne, 1991
299-E34-2	49-50	0.0011	Ames and Serne, 1991
299-E34-2	145-150	0.0000	Ames and Serne, 1991
299-E34-2	230	0.0006	Ames and Serne, 1991
299-E34-3	49-50	0.0004	Ames and Serne, 1991
299-E34-3	119-120	0.0012	Ames and Serne, 1991
299-E34-3	120	0.0065	Ames and Serne, 1991
299-E34-3	164-165	0.0005	Ames and Serne, 1991
299-E34-3	210	0.0000	Ames and Serne, 1991
299-W7-2	64-65	0.0000	Ames and Serne, 1991
299-W7-2	94-95	0.0000	Ames and Serne, 1991
299-W7-2	155	0.0003	Ames and Serne, 1991
299-W7-2	220	0.0000	Ames and Serne, 1991
299-W7-3	450	0.0001	Ames and Serne, 1991
299-W7-5	10	0.0012	Ames and Serne, 1991
299-W10-13	45	0.0008	Ames and Serne, 1991
299-W10-13	115	0.0002	Ames and Serne, 1991
299-W10-13	160	0.0038	Ames and Serne, 1991
299-W10-13	160	0.0003	Ames and Serne, 1991
299-W10-13	200	0.0002	Ames and Serne, 1991
299-W10-13	240	0.0001	Ames and Serne, 1991
299-W10-14	440	0.0002	Ames and Serne, 1991
299-W15-16	40	0.0010	Ames and Serne, 1991
299-W15-16	110	0.0000	Ames and Serne, 1991
299-W15-16	149-150	0.0018	Ames and Serne, 1991
299-W15-16	225	0.0001	Ames and Serne, 1991
299-W15-17	425	0.0091	Ames and Serne, 1991
299-W15-17	425	0.0003	Ames and Serne, 1991
299-W18-21	40	0.0000	Ames and Serne, 1991
299-W18-21	40	0.0051	Ames and Serne, 1991
299-W18-21	94-95	0.0000	Ames and Serne, 1991

299-W18-21	139-140	0.0004	Ames and Serne, 1991
299-W18-21	210	0.0002	Ames and Serne, 1991
299-W18-22	429-431	0.0004	Ames and Serne, 1991
TBS-1	1	0.0002	Serne et al. 1993
MSG-1	1	0.0002	Serne et al. 1993
CGS-1	1	0.0007	Serne et al. 1993
Trench-8	20	0.0019	Serne et al. 1993

Median	**0.00030**
Average	**0.00094**
Std Dev	**0.00179**

Date: September 29, 2000

To: George Last

From: Kenneth Krupka

Subject: **K_d Values for Composite Analysis**

ILAW-PA Geochemical Data Package

K_d Values

The best K_d estimate and range K_d estimate values reported by Kaplan and Serne (1999)[4] in the ILAW-PA geochemical data package were reviewed and compared to those used in the 200 Area Plateau composite analysis by Kincaid et al. (1998).[5] Kaplan and Serne (1999) categorize their K_d values according to five geochemical zones and associated solid and aqueous phases. These geochemical zones are tabulated in Table 1.

The geochemical Zones 3 and 4 used in ILAW-PA geochemical package appear to closely correspond to the "intermediate impact (F)" zone for the "low organic/low salt/near neutral" source category used for the 200 Area composite analysis. The geochemical Zone 5 in ILAW-PA package closely corresponds to the "groundwater (C)" zone for the "low organic/low salt/near neutral" source category used for the 200 Area composite analysis. The best K_d estimate and range K_d estimate values reported by Kaplan and Serne (1999) for Zones 3, 4, and 5 are listed in Table 2 along with the corresponding values from the 200 Area composite analysis for the "low organic/low salt/near neutral" source category.

Geochemical Zone 1 from the ILAW-PA package, which represents a high pH, high ionic strength, glass leachate, may be considered similar to the "high impact (D)" zone for the "very high salt/very basic" source category used in the 200 Area composite analysis. The best K_d estimate and range K_d estimate values reported by Kaplan and Serne (1999) for Zone 1 are listed in Table 3 along with the corresponding values for the "high impact (D)" zone for the "very high salt/very basic" source category from the 200 Area composite analysis.

There appears to be no equivalency between geochemical Zone 2 from the ILAW-PA package, which represents a high pH, high ionic strength concrete leachate, and any of the zones-source categories used in the 200 Area composite analysis.

Kaplan and Serne (1999) noted that "*Essentially all K_d values in the literature and that have been measured at the Hanford Site were generated from sediments that do not contain any*

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[4] Kaplan, D. I., and R. J. Serne. December 20, 1999. *Geochemical Data Package for the Hanford Immobilized Low-Activity Tank Waste Performance Assessment* (ILAW-PA). HNF-5636 Rev. 0 (PNNL-13037), Pacific Northwest National Laboratory, Richland, Washington.

[5] Kincaid, C. T., and others. 1998. *Composite Analysis for Low-level Waste Disposal in the 200 Area Plateau of the Hanford Site*. PNNL-11800, Pacific Northwest National Laboratory, Richland, Washington.

gravel, particles >2-mm." They reviewed the various approaches to correcting K_d values in a gravel dominated sequence. Kaplan and Serne used the following equation for $K_{d(gc,g=0)}$ (gravel-corrected K_d) values:

$$K_{d(gc,g=0)} = (1-f)K_{d(<2mm)}$$

where f was assigned a value of 0.9. Thus Kaplan and Serne decreased all K_d values by an order of magnitude for those values assigned to the gravel-dominated sequence [see Appendix A in Kaplan and Serne (1999)].

Recommendations

Best K_d Estimate Values - Given the limited extent of geochemical conditions represented in the ILAW-PA data package when compared to the number of zones and source categories considered for the 2000 Area composite analysis, it is recommended at this time that the best K_d estimate values used in the ILAW-PA package not be used for composite analyses conducted in the near term. Because only one or two years separated the formulation of these K_d data packages, it has been assumed that two sets of best K_d estimate values were conceptualized differently and therefore best not be mixed.

Range K_d Estimate Values - It is recommended that the ILAW-PA range K_d estimate values be considered for future composite analyses in those cases where the minimum or maximum K_d range values for Zones 1, 3, 4, and 5 are, respectively, less than or greater than the corresponding K_d range estimates previously used for the analogous source-zone categories in the composite analysis. This would result in more conservative ranges for the K_d values for each contaminant.

Gravel vs. Sand Sequence K_d Values – Until additional information or experimental results are available, it is recommended that the gravel K_d correction described in Appendix A in Kaplan and Serne (1999) be used for gravel sequence calculations that are part of future composite analyses.

K_d Values for Carbon Tetrachloride

Kirk Cantrell (PNNL) describes the results of a review of K_d values for carbon tetrachloride in the memorandum "Estimation of the Carbon Tetrachloride Adsorption Coefficient for Hanford Sediments" to George Last on August 3, 2000. Based on this review, Cantrell "*estimated that the most probably value for a K_d for carbon tetrachloride adsorption onto Hanford sediment is 0.2 mL/g, with a range of approximately 0.1 to 0.6.*"

I have assumed that these values correspond to the "groundwater (C)" zone in the "low organic/low salt/near neutral" source category used in the 200 Area composite analysis. The review does not state how these K_d values relate to the carbon tetrachloride adsorption in the

other zones-source categories used in the 200 Area composite analysis nor how they are affected by the gravel K_d issues and existing correction methods.

K_d Values for Cr(VI) (Chromate)

Based on batch adsorption tests, Serne and Parker[6] conclude that there is no significant adsorption of Cr(VI) onto Hanford Formation sediments. They recommend that "*a K_d value of 0 mL/g continue to be used for future predictive modeling of the fate of Cr(VI) in the 100 Areas.*"

It is recommended that best K_d estimate and range K_d estimate values used for highly-mobile tritium in the different zone-source categories in the 200 Area composite analyses by Kincaid et al. (1998) be used as a surrogate for Cr(VI) (chromate) in future composite analyses until additional information or results from new Cr(VI) adsorption measurements and experimental studies become available.

Distribution Function for K_d Values Within Range K_d Estimates

The topic of distribution functions for the representation of K_d values within range K_d estimates is a subject of continued debate. Most range K_d estimates attempt to capture a range of geochemical conditions, such as variation in ground-water pH conditions and/or differences (or heterogeneities) in the dominant adsorbate(s) present in a geochemical system. Arguments have been made that this variation should be represented by some form of a normal or log-normal distribution function.

I believe that such functions best represent data whose variation is due replication and experimental error during their measurements and not necessarily for representing geochemical heterogeneities in a ground-water/sediment system(s). For example, the general adsorption behavior of an anion or cation as a function of ground-water pH, given all other conditions remain constant, is known and is not random. Therefore, I recommend that, as a most conservative methodology, a constant distribution function be used for representation of K_d values within range K_d estimates, where the probability of a K_d value being equal to the minimum, maximum, or any value between these extremes be equal to "1." This topic, however, will continue be a source of debate.

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6 Serne, R. J., and K. E. Parker. October 28, 1999 (**internal draft**). *Estimation of Distribution Coefficients and Leachability of Hexavalent Chromium in 100-D Area Hanford Formation Sediments*. Draft report prepared for Bechtel Hanford, Inc. by Pacific Northwest National Laboratory, Richland, Washington.

Table-1. Descriptions of five geochemical zones used for ILAW-PA geochemical package. [Information extracted directly from Kaplan and Serne (1999)].

Zone	Solid Phases	Aqueous Phase
Zone 1 – Near Field	Glass, secondary phases formed from glass degradation, and backfill and engineered barrier materials	Glass leachate; high pH, high ionic strength, high radionuclide concentrations
Zone 2- Degraded Concrete Vault	Three assemblages of minerals will exist, based on concrete age	Three types of concrete leachate chemistries controlled by different aged solid phases: fresh concrete with pH=12.5, moderately aged concrete with pH≈10.5, and completely aged concrete with pH≈8.5; generally high in ionic strength and high radionuclide concentrations
Zone 3 – Chemically Impacted Far Field in sand Sequence	Sand-dominated sequence, slightly altered due to contact with moderately caustic aqueous phase	pH 8 (background) to 11; ionic strength 0.01 (background) to 0.1, low radionuclide concentrations
Zone 4 – Chemically Impacted Far Field in Gravel Sequence	Same as Zone 3 except in gravel-dominated sequence	Same as Zone 3 except in gravel dominated sequence
Zone 5 – Far Field in gravel Sequence	Unaltered Hanford gravel sequence (90% gravel, 10% <2-mm)	Unaltered Hanford groundwater except for trace concentrations of radionuclides

Table 2. Source category – Low organic/low salt/near neutral

Element	High Impact (G) Composite Analysis (Kincaid et. al. 1998)		Intermediate Impact (F) Composite Analysis (Kincaid et. al. 1998)[5]		Zone 3 Sand Sequence Geochemical Data Package (Kaplan and Serne 1999)		Zone 4 Gravel Sequence Geochemical Data Package (Kaplan and Serne 1999)		Groundwater (C) Composite Analysis (Kincaid et. al. 1998)		Zone 5 Gravel Sequence Geochemical Data Package (Kaplan and Serne 1999)	
	Best K_d Estimate (mL/g)	Range K_d Estimate (mL/g)	Best K_d Estimate (mL/g)	Range K_d Estimate (mL/g)	Best K_d Estimate (mL/g)	Range K_d Estimate (mL/g)	Best K_d Estimate (mL/g)	Range K_d Estimate (mL/g)	Best K_d Estimate (mL/g)	Range K_d Estimate (mL/g)	Best K_d Estimate (mL/g)	Range K_d Estimate (mL/g)
Highly Mobile Elements												
Tritium	0	-2.8 to 0.6	0	-2.8 to 0.6	0	0 to 0.1	0	0 to 0.01	0	-2.8 to 0.6	0	0 to 0.06
Tc-99	0	-2.8 to 0.6	0	-2.8 to 0.6	0	0 to 0.1	0	0 to 0.01	0	-2.8 to 0.6	0	0 to 0.06
Somewhat Mobile Elements												
I-29	0.5	0.2 to 15	0.5	0.2 to 15	0	0 to 2	0	0 to 0.2	0.5	0.2 to 15	0.01	0 to 1.5
Uranium	3	0.1 to 79.3	3	0.1 to 79.3	10	2 to 500	1	0.2 to 50	3	0.1 to 79.3	0.06	0.01 to 8
Moderately Immobile Elements												
Sr-90	20	5 to 173	20	5 to 173	10	0.2 to 50	1	0.02 to 5	20	5 to 173	1.4	0.5 to 20
Cs-137	300	67 to 1330	300	67 to 1330	80	40 to 2000	8	4 to 200	300	67 to 1330	200	50 to 400
Highly Immobile Elements												
Pu-239/240	200	80 to >1980	200	80 to >1980	200	80 to 1000	20	8 to 100	200	80 to >1980	15	5 to 200
Organic Elements												
Carbon Tetrachloride												
Inorganic Elements												
Cr												

Attachment 3B

Table 3. Source category – very high salt/very basic

Element	High Impact (G)		Zone 1 Near Field	
	Composite Analysis (Kincaid et. al. 1998)		Geochemical Data Package (Kaplan and Serne 1999)	
	Best K_d Estimate (mL/g)	Range K_d Estimate (mL/g)	Best K_d Estimate (mL/g)	Range K_d Estimate (mL/g)
Highly Mobile Elements				
Tritium	0	0 to 0.2	0	0 to 1.1
Tc-99	0	0 to 0.2	1	0.1 to 1.2
Somewhat Mobile Elements				
I-29	0	0 to 0.2	0	0 t 1.1
Uranium	20	10 to 800	20	10 to 800
Moderately Immobile Elements				
Sr-90	10	4 to 20	10	4 to 20
Cs-137	1.5	1 to 25	1.5	1 to 25
Highly Immobile Elements				
Pu-239/240	10	5 to 100	10	5 to 100
Organic Elements				
Carbon Tetrachloride				
Inorganic Elements				
Cr				

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Project No.

Internal Distribution
AL Bunn
PW Eslinger
DG Horton
CT Kincaid
WE Nichols
RJ Serne

Date	May 10, 2001
To	Distribution
From	George Last and Kirk Cantrell
Subject	<u>Kd Distributions for SAC Rev. 0</u>

cc:
KM Krupka
RG Riley

This memo is a follow up to our meeting of December 18, 2000, and address three main issues: 1) how to deal with negative Kd values, 2) the probability distribution of Kd values within a given range, and 3) re-examination of the some of the extremely high Kd values.

<u>Issue 1 - Negative Kd values</u>.
In our December 18 meeting we all agreed that the Kd ranges should be truncated at zero, so that we have no negative Kds.

<u>Issue 2 - Probability Distribution of Kd Values</u>
We also discussed the impact of truncating the Kd ranges where the best estimate is zero and range may have contained negative numbers. This would bias the Kd range toward higher sorption. Thus, we agreed that for those contaminants (i.e., H^3, Tc^{99}, and Cr) we would assume a constant of zero (no range or distribution).

As for the other contaminants, we have since re-examined the use of uniform vs log-normal probability distributions for Kd values within a given range. Defensible rational for any type of probability distribution was not readily found. Ken Krupka had earlier recommended the use of a uniform distribution since all values had to be taken as having equal weight at this time (without detailed examination/review). However, the *Geochemical Data Package for the ILAW PA* (Kaplan and Serne 2000), assumed a log-normal distribution, and the *Stochastic Parameter Development for PORFLOW Simulations of the Hanford AX Tank Farm* (Clifford, et. al. 1999) assumed a log-uniform distribution. After much debate and consternation we recommend using the log-normal distribution (as generally agreed to in our December 18 meeting). This is more consistent with the most recent stochastic approaches used at Hanford; is more intuitively reasonable (due to the otherwise severe bias effected by some the very high [and questionable] Kd values); and would likely give more conservative results (i.e.,lower adsorption). Per our discussions on December 18, the log-normal distribution would be defined by the median (actually the best guess value), and the minimum value (taken as the lower bound). A revised Kd table for use in SAC Rev. 0 is attached.

<u>Issue 3 - Extremely High Kd Values</u>

We have reviewed the data sources for some the extremely high Kd values present in the proposed Kd ranges and have found that many of these are due to precipitation effects. However, at this time we can not defensibly throw out any of these data.

Recommendations for SAC Rev. 1
The current "data base" of Kd values, represents a real hodge-podge of analyses, conducted at different times, with different methodologies (e.g. batch vs column), different concentrations, different water types (major ion concentrations), different pH, different soils, , etc. In some cases, the tabulated Kd values describes a combination of adsorption as well as precipitation phenomena. A Kd approach is not an appropriate model for the description of solubility phenomena and values determined under such conditions should not be used. Thus, the current selection of the most appropriate Kd, ranges, and probability distributions, can not be rigorously defended. Additional review, evaluation, documentation, and regrouping of the current data, along with supplemental testing (particularly for those contaminants with low Kds), will be needed to provide a defensible position for SAC Rev. 1, and for other near term assessments as well. Refer to the proposal "Proposed Scope of Work to Revise and Update the Hanford Site's Contaminant Distribution Coefficient Databases and Develop Spatial Hydrostratigraphic/Geochemical Correlations" dated August 2000.

References:
Clifford, K. H., et. al., 1999. Stochastic Parameter Development for PORFLOW Simulations of the Hanford AX Tank Farm. SAND98-2880. Sandia National Laboratories, Albuquerque, NM.

Kaplan, D. I., and R. J. Serne. 2000. Geochemical Data Package for the Hanford Immobilized Low-Activity Tank Waste Performance Assessment (ILAW-PA). PNNL-13037, Rev. 1, Pacific Northwest National Laboratory, Richland, WA.

Kincaid, C. T., et. al. 1998. Composite Analysis for Low-Level Waste Disposal in the 200 Area Plateau of the Hanford Site. PNNL-11800. Pacific Northwest National Laboratory, Richland, WA.